Chilwerth

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Property Data for CFD Fire Models
(Heat of Gasification of Wood Materials)

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Objectives

- Develop techniques for measuring the heat of gasification
- Conduct experiments which would provide a better understanding of the heat of gasification and lead to a method of calculating it
- Develop a procedure for incorporating heat of gasification in CFD models

The first objective is discussed in this presentation

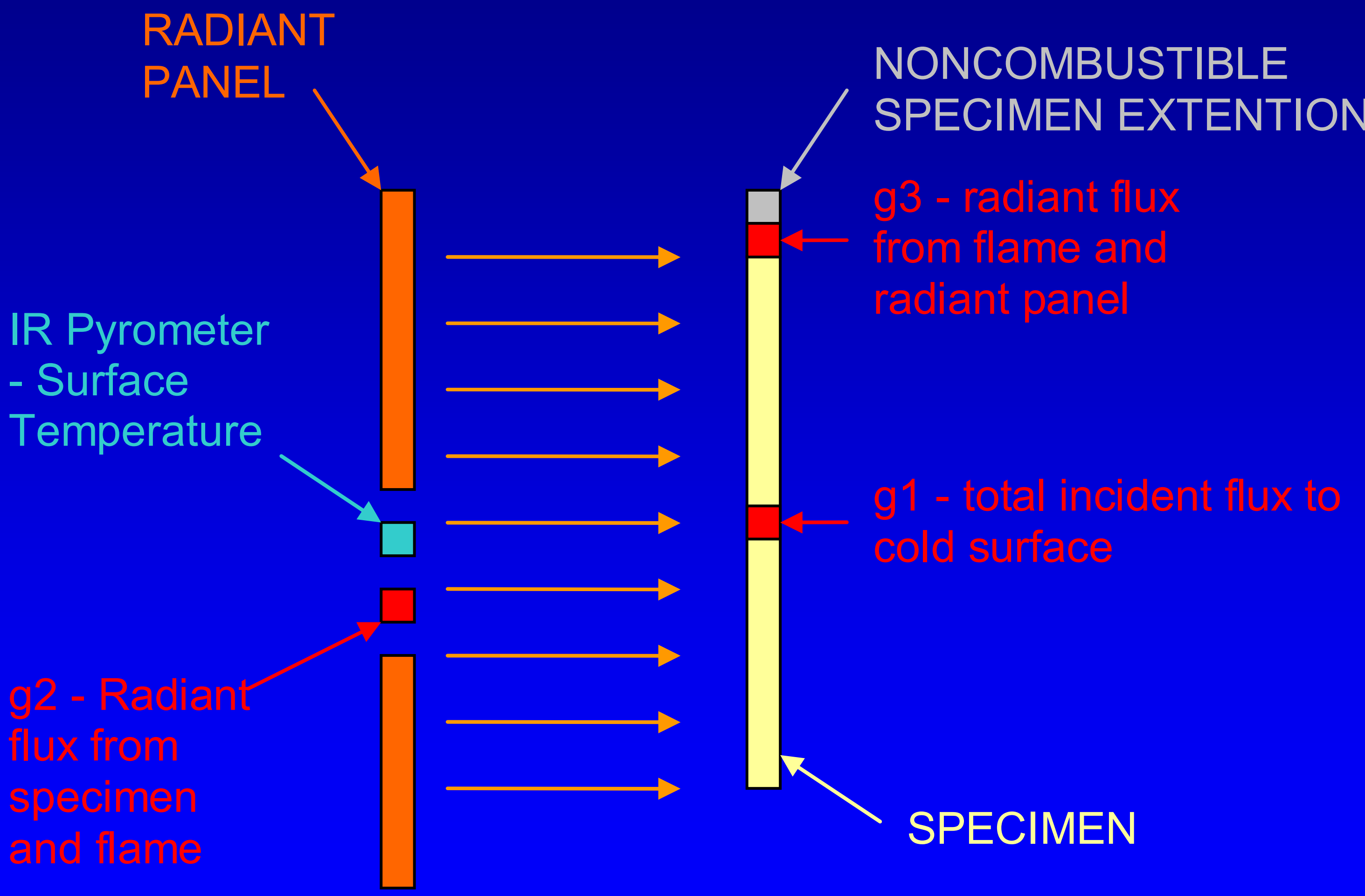
INTRODUCTION

- A standard calorimeter measures heat release rate as a function of incident flux
- The fire performance of a material is a function of net heat flux
- The mass flow of volatile pyrolysis products out through surface is given by:

$$\dot{m}''_{vol} = \frac{\dot{q}''_{net}}{h_g}$$

- To determine the heat of gasification it is necessary to measure the net heat flux

Direct Measurement Based on Net Heat Flux and Mass Loss Rate Measurement (1)

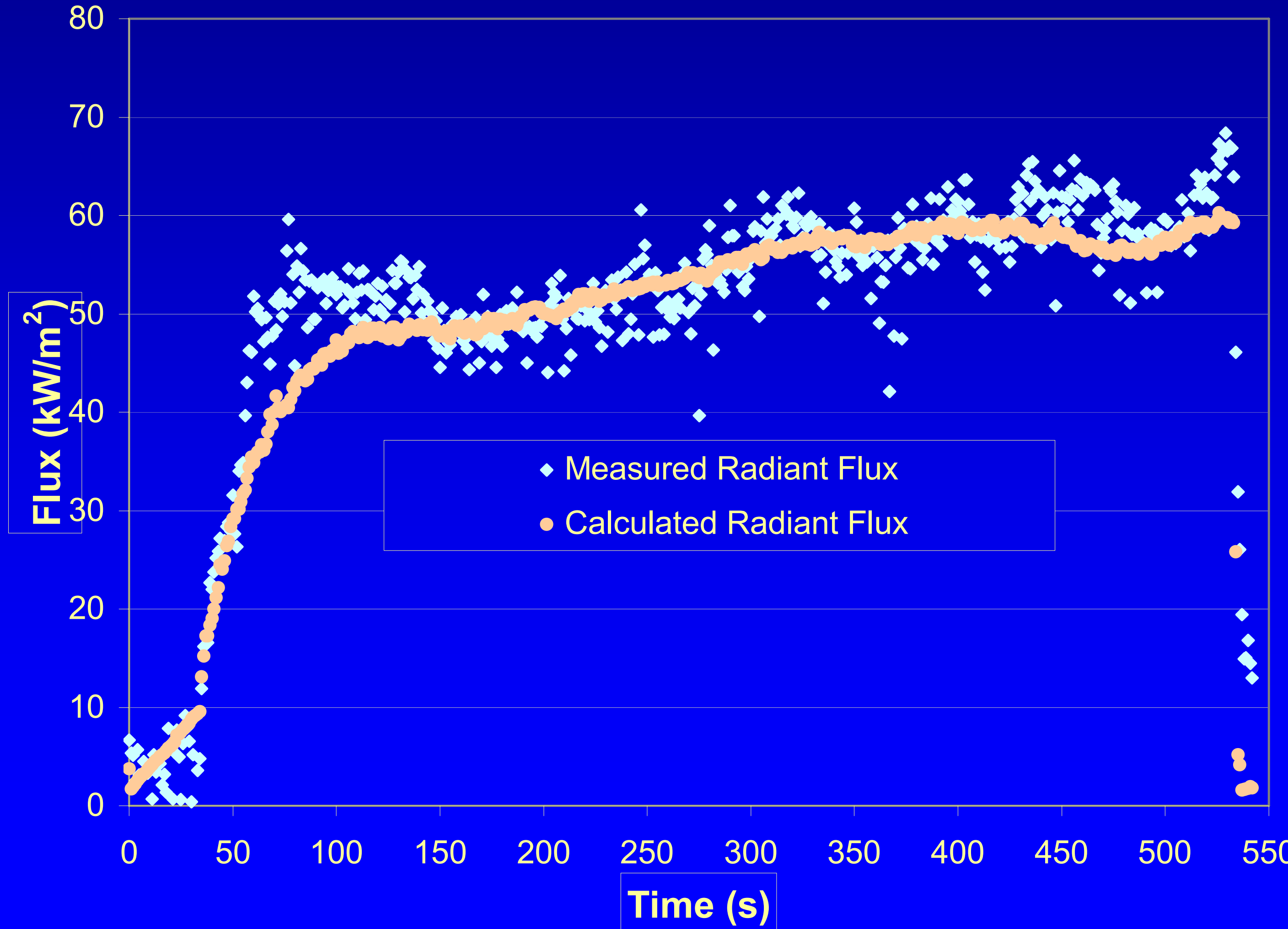


Direct Measurement Based on Net Heat Flux and Mass Loss Rate Measurement (2)
Technique 1

- The calculated radiation loss from the surface replaced the measured value when it was found that good agreement was obtained by using an emissivity setting of 1.0.

Direct Measurement Based on Net Heat Flux and Mass Loss Rate Measurement (3)

Technique 1 – Comparison of the Measured and Calculated Radiation Emitted by the Surface (Particleboard at 50 kW/m^2)



Direct Measurement Based on Net Heat Flux and Mass Loss Rate Measurement (4)

$$h_g = \frac{\dot{q}''_{net}}{\dot{m}''_{vol}}$$

- Measurements were made in the ICAL
- Three techniques were developed for direct net heat flux measurement:
  1. Measured total incoming flux and surface temperature

     $$\dot{q}''_{net} = q''_{g1} - \sigma\varepsilon(T_s^4 - T_0^4) - \xi h_1(T_s - T_{g1})$$

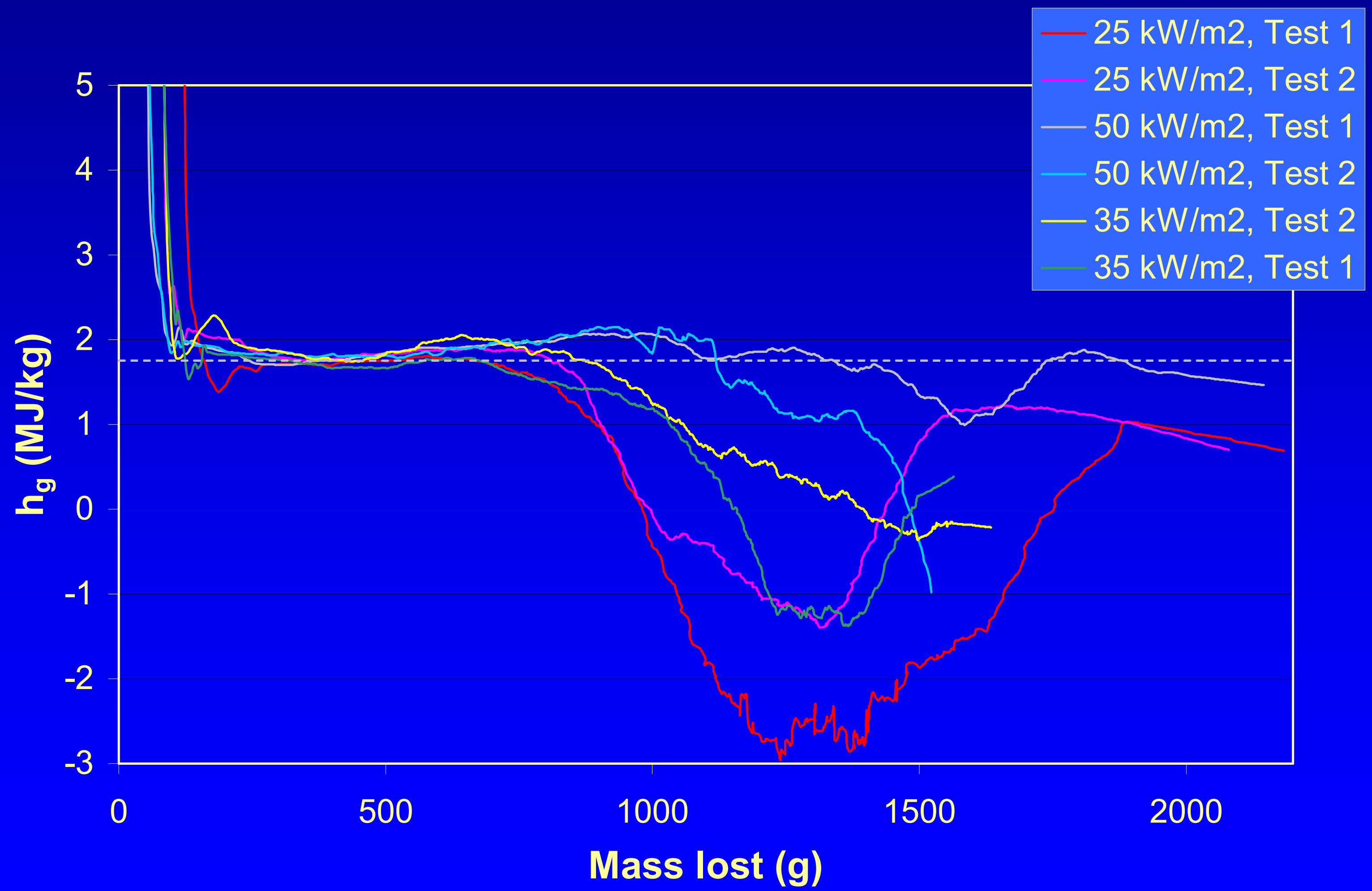
  2. Measured total incoming radiation and surface temperature; convection measured on non-combustible board and multiplied by the blowing factor

     $$\dot{q}''_{net} = \dot{q}''_{g4} + \xi\dot{q}''_{cv} - \sigma\varepsilon(T_s^4 - T_\infty^4)$$

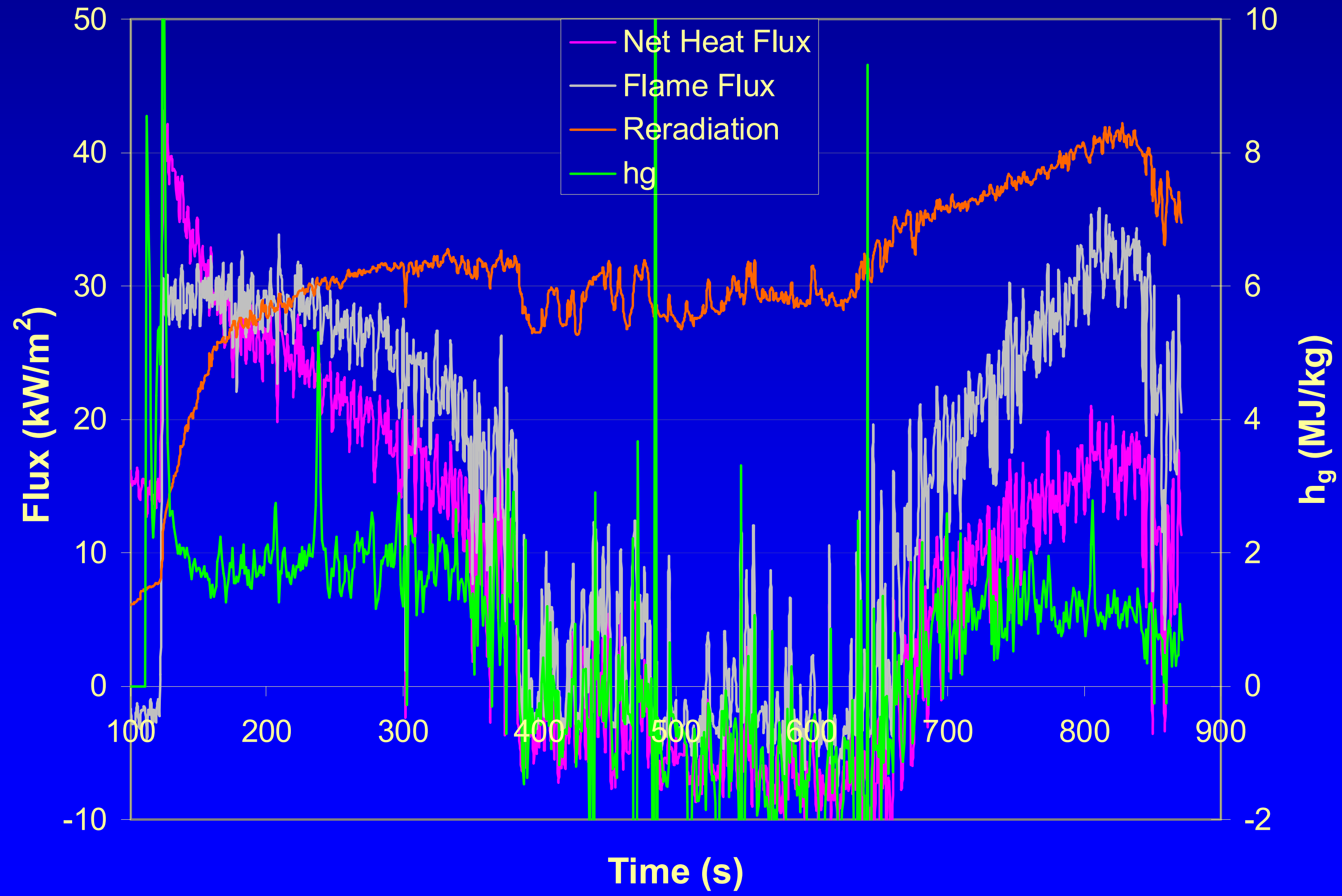
  3. Used natural gas flame, on non-combustible board pre-measured flame radiation (PMFR), calculated convection, and measured surface temperature

$$\dot{q}''_{net} = PMFR + \dot{q}''_{ext} + \xi\dot{q}''_{cv} - \sigma\varepsilon(T_s^4 - T_\infty^4)$$

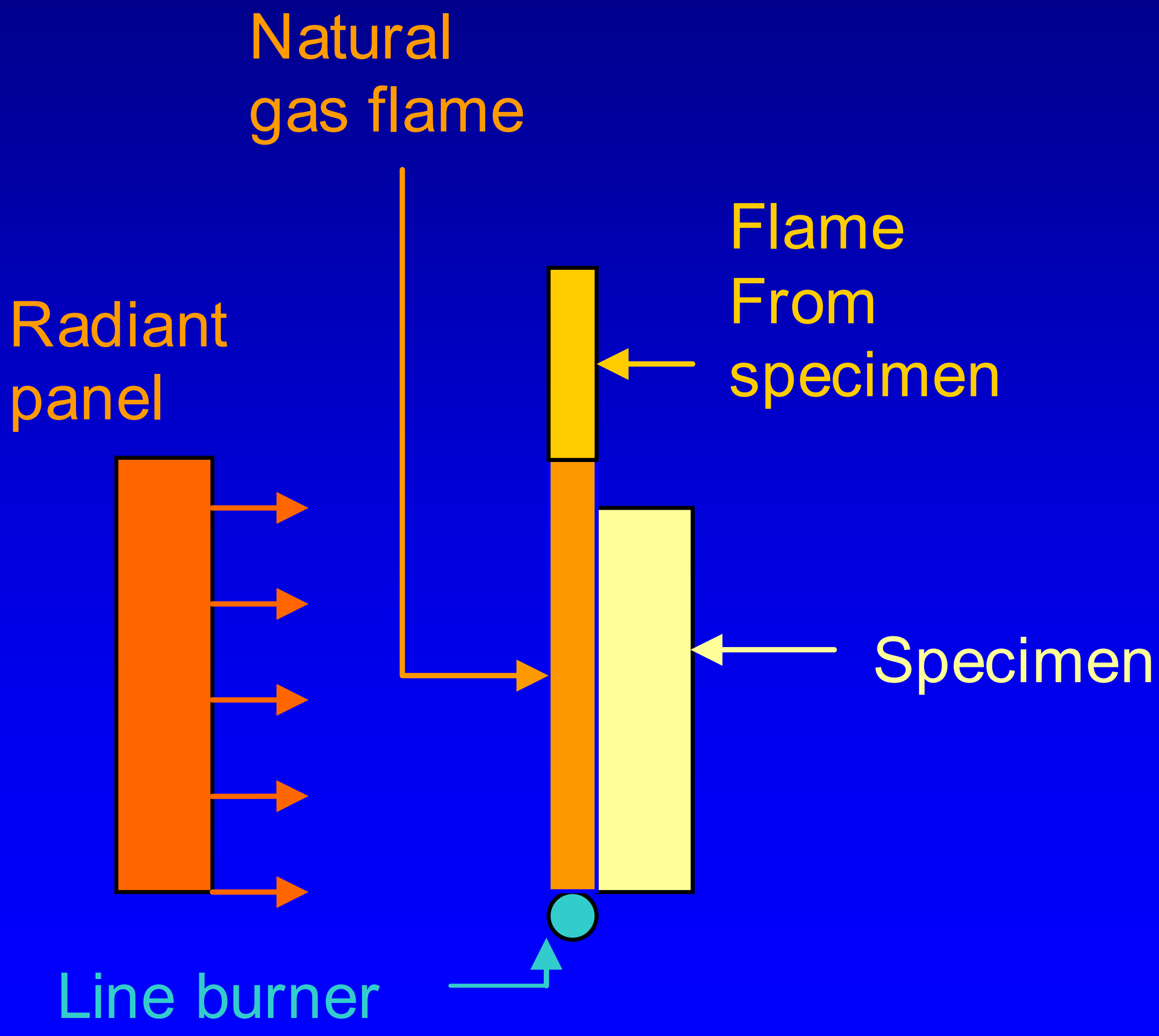
Results
Measured Heat of Gasification (1)
Particleboard – Technique 1



Results
Measured Heat of Gasification
Particleboard at 25 kW/m^2– Net Heat Flux, Flame Flux, Re-radiation, and Heat of Gasification

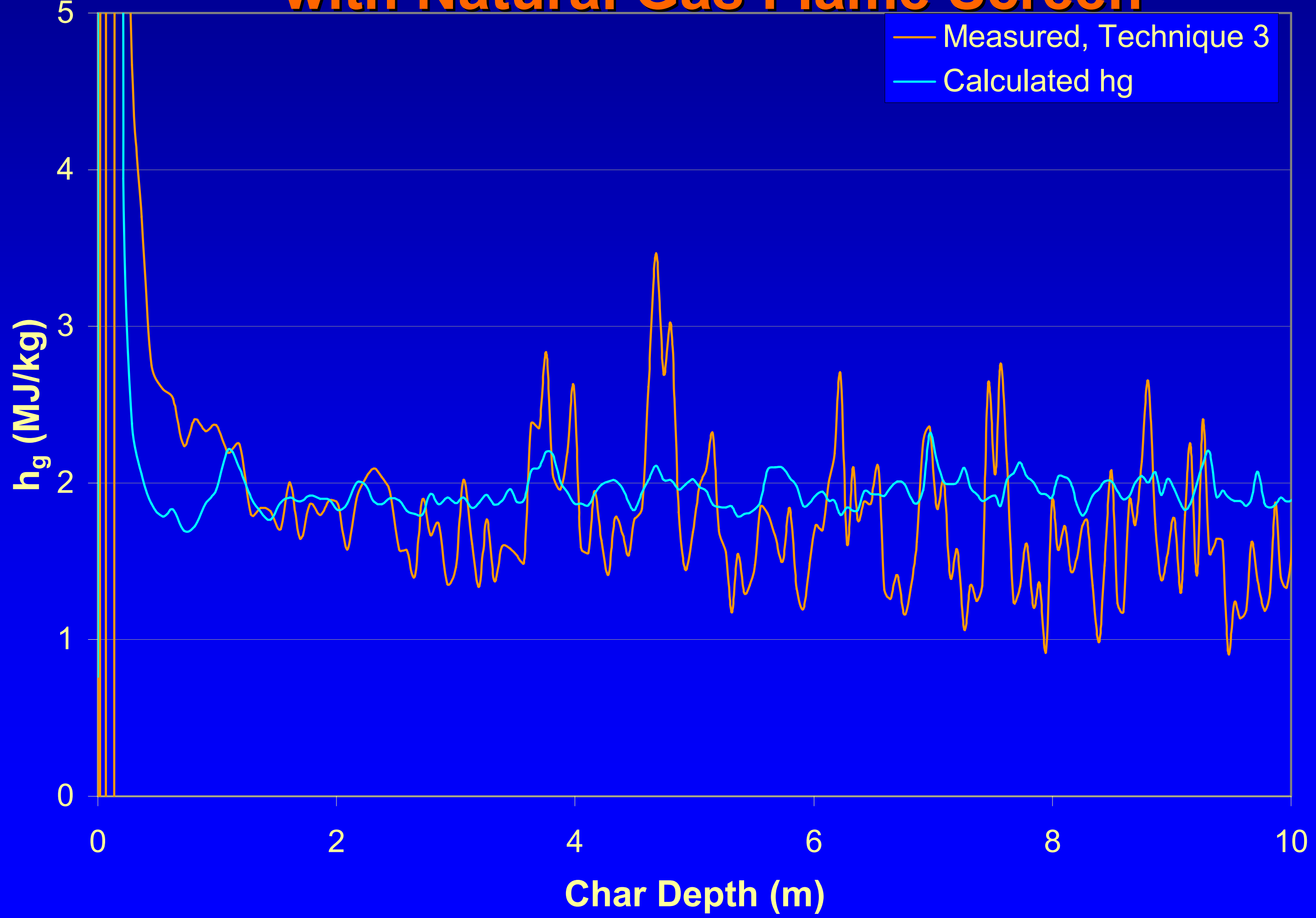


Measured Heat of Gasification
Technique 3



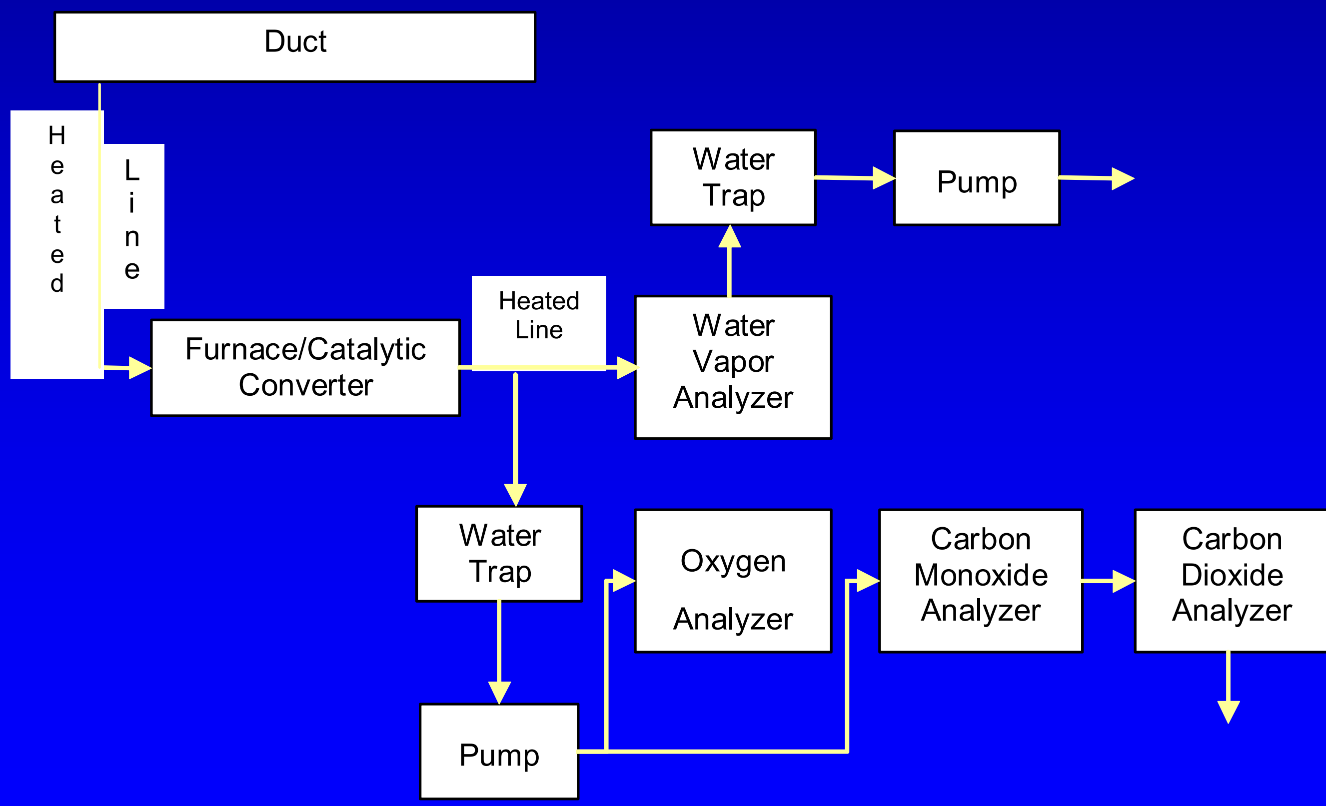
Results
Measured and Calculated Heat of Gasification

Douglas Fir at 15 kW/m²–Calculated and Measured h_g with Natural Gas Flame Screen



Measurements of C, H, and O in the Volatile Pyrolysis Products (1)

- Measure X_{H2O}, X_{CO2}, X_{O2} in analyzers



Measurements of C, H, and O in the Volatile Pyrolysis Products (2)

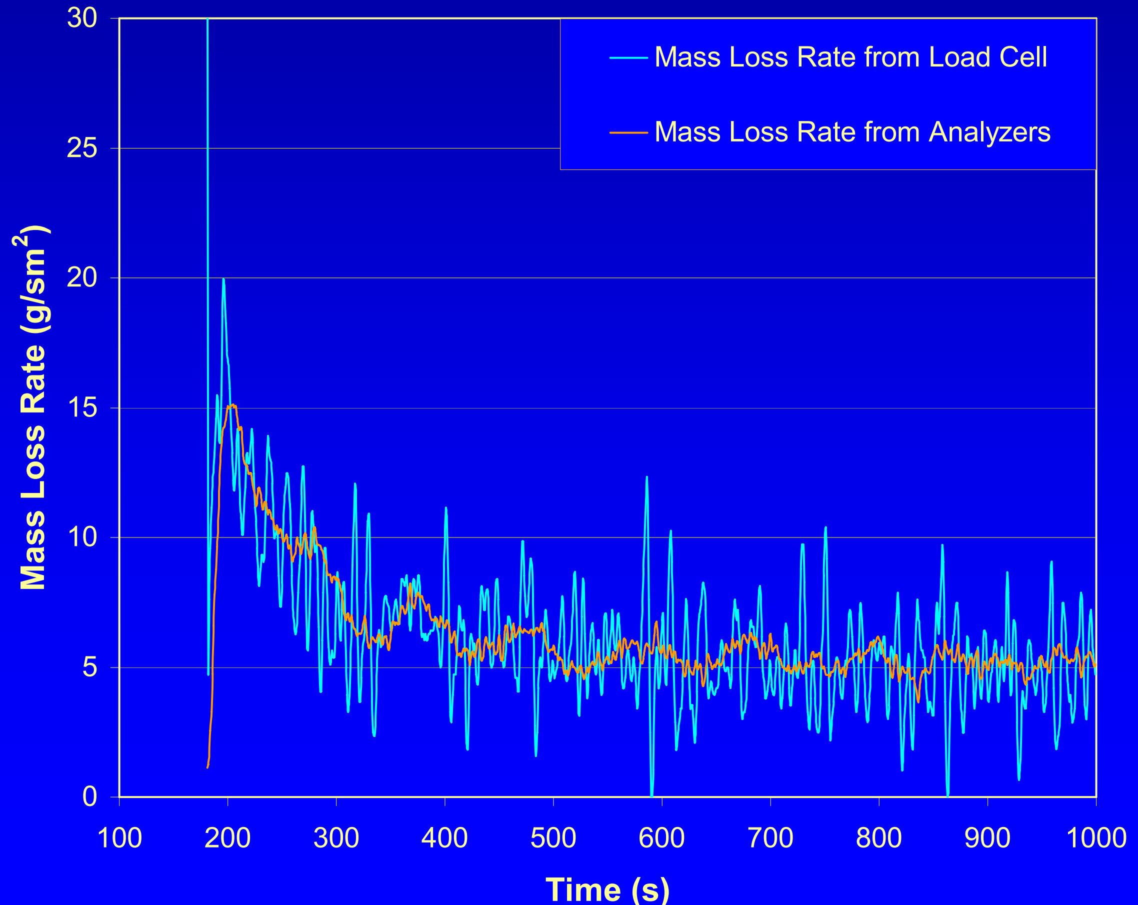
- All of the C atoms are oxidized to CO_2
- All of the H atoms are oxidized to H_2O
- For every 44 grams of CO_2 measured there are 12 grams of <u>C atoms</u> in the volatiles.
- For every 18 grams of H_2O measured there are 2 grams of <u>H atoms</u> in the volatiles
- The mass of O_2 required to oxidize the C and H atoms minus the grams of O2 consumed is equal to the mass of <u>O atoms</u> in the volatiles

Measurements of C, H, and O in the Volatile Pyrolysis Products (3)

- The total mass flows of the C, H, and O atoms from a specimen is equal to the mass loss rate of the specimen
- Using these mass flows, the rate of char production, rate of pyrolysis, char depth and mass flow of absorbed water from a wood specimen can be determined as a function of time. These parameters are needed to calculate the heat of gasification as a function of char depth if the specimen has a significant moisture content.
- 13.1 MJ/kg times the O_2 consumption divided by the mass loss rate is equal to the heat of combustion

Calculation of Mass Loss Rate Based on Measurements of C, H, and O in the Volatile Pyrolysis Products (3)

$$\dot{m}^{spec} = \dot{m}_C^{spec} + \dot{m}_H^{spec} + \dot{m}_O^{spec}$$



Summary

- Three techniques were developed for direct h_g measurements
- For direct h_g measurements the specimen must be completely covered with flame
- Only the technique using the natural gas can provide full flame coverage over the complete test. Even for extremely high incident fluxes there will still be a problem near the end for the first two techniques.
- Individual mass flows of C, H, and O in volatile pyrolysis products can be determined by adding a catalytic converter and H_2O analyzer to a HRR calorimeter

$$\dot{m}_{vol}^{''} = \frac{\dot{q}_{net}^{''}}{h_g}$$

Discussion of Heat of Gasification (1)

- **Definition of "measured" heat of gasification"**

$$\dot{m}_{vol}^{''} = \frac{\dot{q}_{net}^{''}}{h_g}$$

- **Overall formula for heat of gasification (when broken down)**

$$h_g = \alpha h_g^I + \beta h_S + h_T + h_{loss}$$

$h_g^I - Interior\ h_g$

$\alpha = 1/(1-R)$

$h_S - Heat\ of\ storage$

$\beta = R/(1-R)$

$h_T - Heat\ of\ transit$

$h_{loss} - Heat\ loss\ coefficient\ (\frac{\dot{q}_{loss}^{''}}{\dot{m}_{vol}^{''}})$

$R - Char\ fraction\ (rate\ of\ char\ production\ divided\ by\ rate\ of\ pyorlysis)$

Discussion of Heat of Gasification (2)

Interior Heat of Gasification

$$h_g^I = h_{pyr} + \overline{C}_{wood}\left(T_{pyr} - T_0\right)$$

Heat of Storage

$$h_S = \overline{c}_{char}(T_S - T_{pyr})$$

Heat of Transit

$$h_T = \overline{c}_{vol}(T_S - T_{pyr})$$

Calculation of Heat of Gasification Based on Measurements of C, H, and O in the Volatile Pyrolysis Products (1)

- **Calculate molar flows of H_2O, CO_2, and O_2 from specimen by taking the gases produced by combustion of ICAL natural gas and ambient gases into account:**

$$\dot{n}_{H2O}^{spec} = X_{H2O}\dot{n}_T - \dot{n}_{H2O}^{air} - \dot{n}_{H2O}^{gas}$$

$$\dot{n}_{CO2}^{spec} = X_{CO_2^*}\dot{n}_T - \dot{n}_{CO2}^{air} - \dot{n}_{CO2}^{gas}$$

$$\dot{n}_O^{spec} = 2\dot{n}_{CO2}^{gas} + \dot{n}_{H2O}^{gas} + 2\dot{n}_{CO2}^{spec} + \dot{n}_{H2O}^{spec} - 2(X_{O2}^0 - X_{O2})\dot{n}_T$$

$$\dot{n}_C^{spec} = \dot{n}_{CO2}^{spec}$$

$$\dot{n}_H^{spec} = 2\dot{n}_{H2O}^{spec}$$

$$\dot{m}_C^{spec} = 12\dot{n}_C^{spec}$$

$$\dot{m}_H^{spec} = \dot{n}_H^{spec}$$

$$\dot{m}_O^{spec} = 16\dot{n}_O^{spec}$$

Calculation of Heat of Gasification Based on Measurements of C, H, and O in the Volatile Pyrolysis Products (2)

- **Rate of char production** is mass flow of carbon into pyrolysis zone minus mass flow of carbon in the duct. Assuming none of hydrogen is going into the char:

$$\dot{m}_{Char} = [(\dot{m}_C / \dot{m}_H)^0 - (\dot{m}_C / \dot{m}_H)]\dot{m}_H$$

- **Rate of pyrolysis** is the mass flow of the original material into the pyrolysis zone:

$$\dot{m}_{pyr} = \dot{m}_{char} + \dot{m}_{vol}$$

- **Char fraction:**

$$R = \dot{m}_{char} / \dot{m}_{pyr}$$

All of the above is for a dry specimen

Calculation of Heat of Gasification Based on Measurements of C, H, and O in the Volatile Pyrolysis Products (3)

- **Char depth** if char fraction is constant:

$$\delta = \frac{M}{\rho(1-R)}$$

otherwise:

$$\delta = \frac{1}{\rho}\int_0^t \dot{m}_{pyr}\,dt$$

Calculation of Heat of Gasification Based on Measurements of C, H, and O in the Volatile Pyrolysis Products (4)

- **Dealing with absorbed moisture – calculating the rate of pyrolysis as if the specimen were dry:**
  - **Hydrogen:**

$$\dot{m}_H^{abs} = \dot{m}_C\left(\left(\frac{\dot{m}_H}{\dot{m}_C}\right) - \left(\frac{\dot{m}_H}{\dot{m}_C}\right)^*\right)$$

  - **Water:**

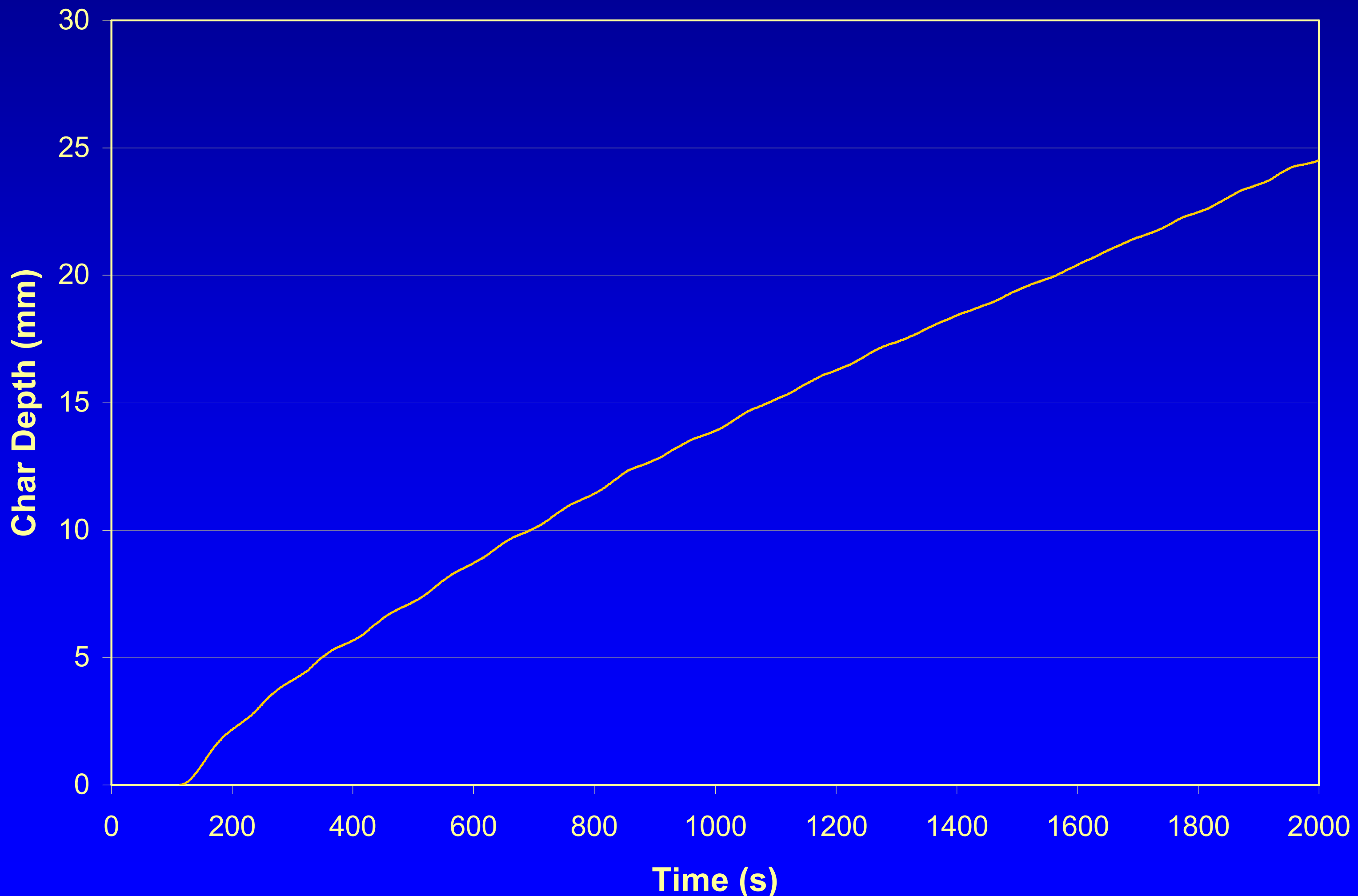
$$\dot{m}_{H_2O}^{abs} = 9 \times \dot{m}_H^{abs}$$

  - **Rate of pyrolysis:**

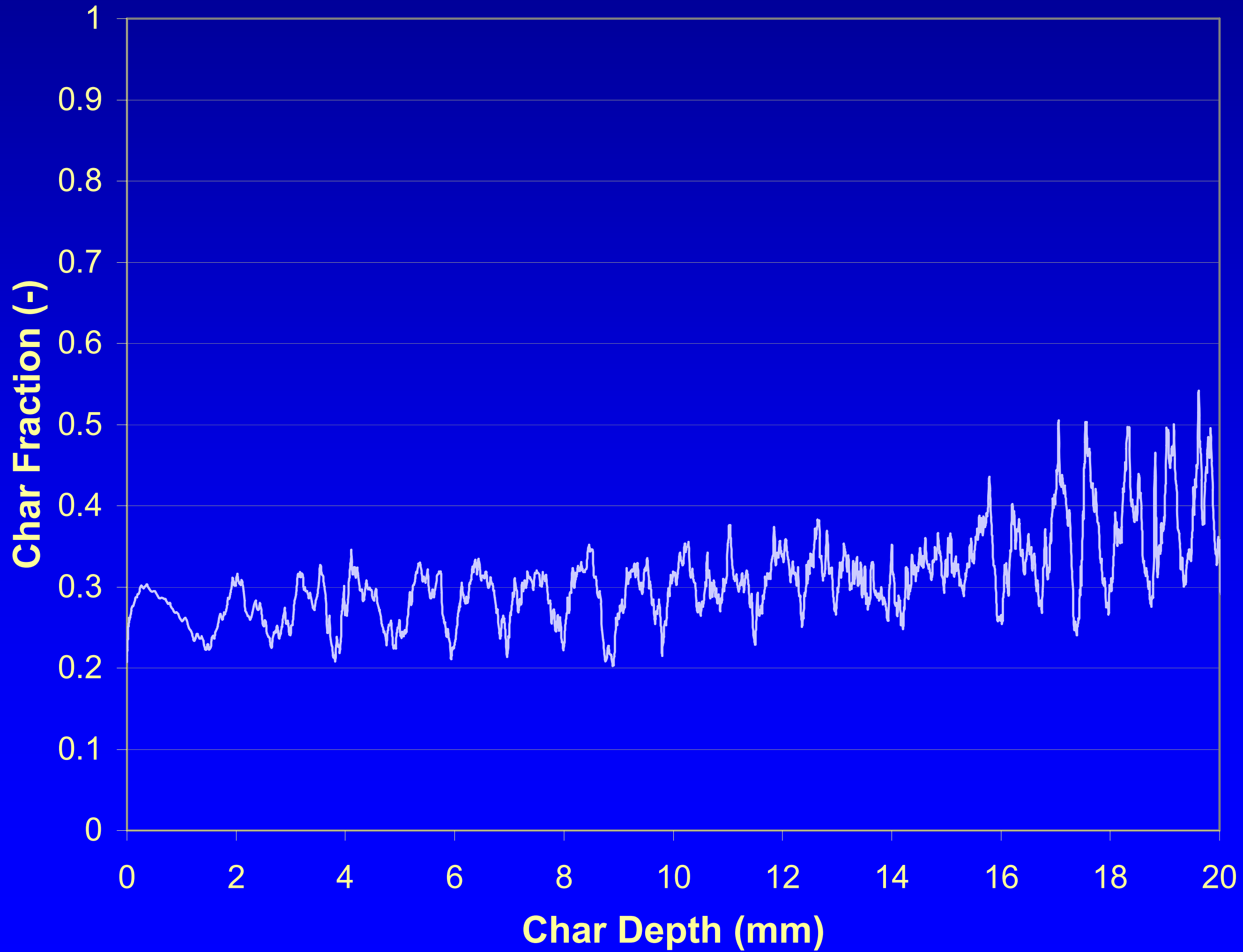
$$\dot{m}_{pyr} = \dot{m}_{char} + \dot{m}_{vol} - \dot{m}_{H_2O}^{abs}$$

Results
Measured Heat of Gasification (2)
Douglas fir at 35 kW/m^2 after 10 minutes

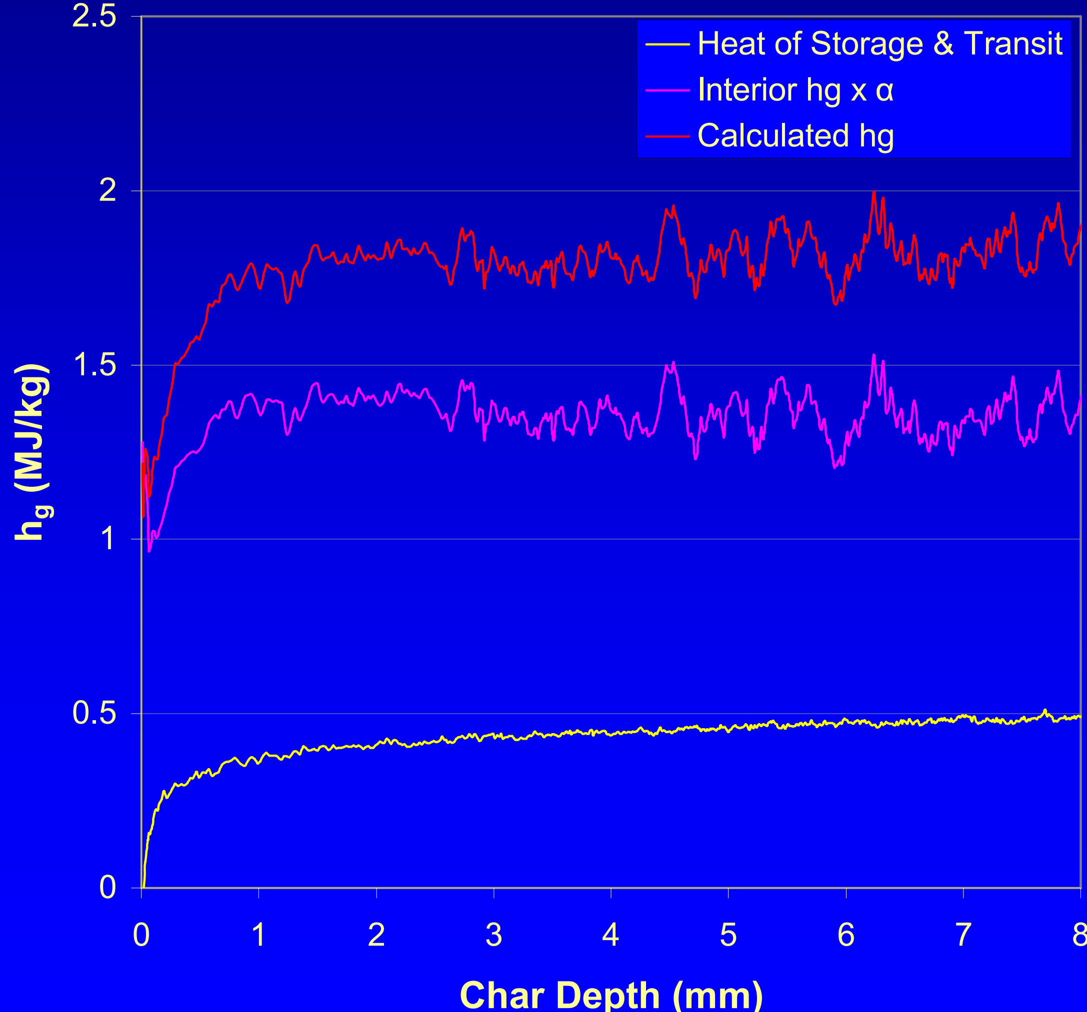
Results
Calculated Heat of Gasification (1)
Douglas Fir at 35 kW/m^2– Char Depth v. Time



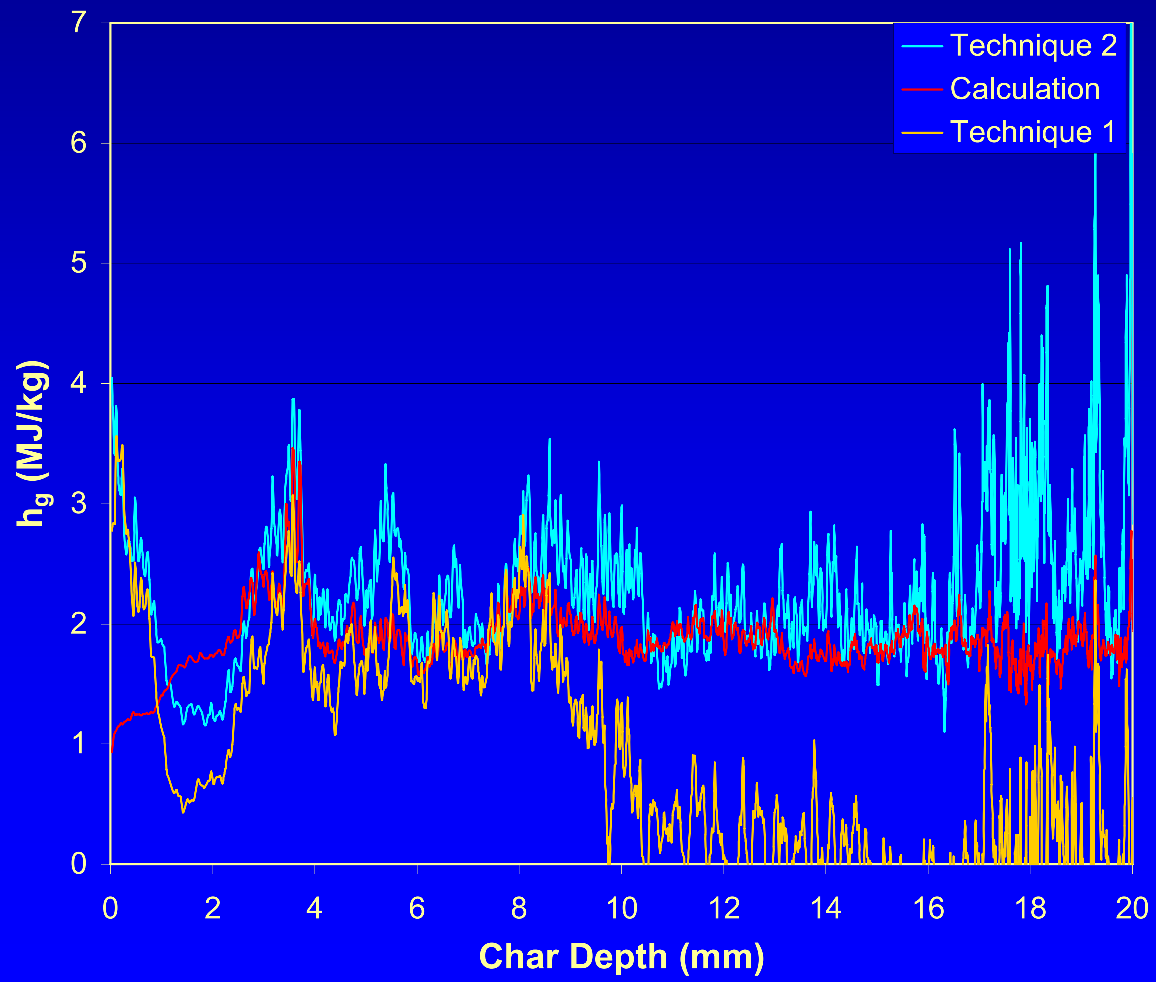
Results
Calculated Heat of Gasification (2)
Douglas Fir at 35 kW/m^2– Char Fraction



Results
Calculated Heat of Gasification (3)
Douglas Fir at 35 kW/m^2– Heat of Storage & Transit, Interior h_g, Calculated h_g



Results
Calculated Heat of Gasification (4)
Douglas Fir at 35 kW/m^2–Calculated and Measured h_g



Inclusion into CFD Model (1)

- The tested materials would have to have the same thickness and rear boundary conditions
- Heat of gasification would need to be measured as a function of char depth
- The model would have to predict char depth:

  M is accumulated mass predicted up to the time step

  R is char fraction, ρ is density of original material

$$\delta = \frac{M}{\rho(1-R)}$$

- Char fraction and h_g are given to the model (polynomials if not constant)
- CFD model would calculate net heat flux and use the above equation to predict mass loss rate
- Surface temperature needs to be calculated by the model
- The model needs to recognize when flaming can no longer be supported

Inclusion into CFD Model (2)

Need for the Same Thickness and Rear Surface Boundary Conditions

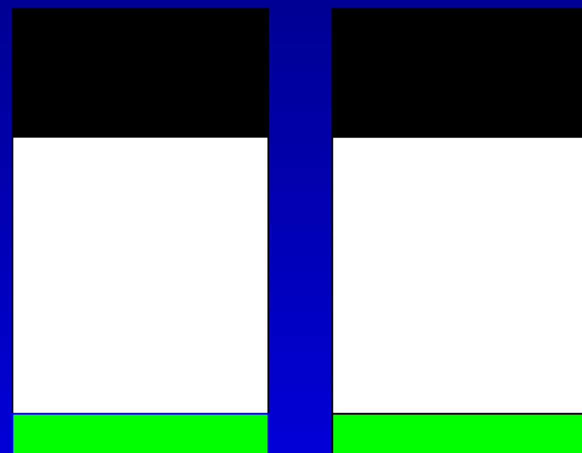
Section of wall in a room

Specimen in a laboratory

Same char depth

Same properties

Same thickness



Same boundary condition

Same heat of gasification

Entirely different mass loss rate histories - This can only be due to the different heat fluxes

$$\dot{m} = \dot{q}_{net} / h_g$$

This is why the boundary condition must be the same and the transfer of information must be made at the same char depth so that the heat of gasification is the same for the wall and the specimen

Summary (2)

- Heat of gasification defined as net heat flux divided by mass loss rate includes:
  - Interior heat of gasification
  - Heat of storage
  - Heat of transit
  - Heat loss coefficient

Summary (3)

- Heat of gasification can be calculated as a function of char depth.
  - Interior h_g was calculated by assuming the heat of pyrolysis to be zero and pyrolysis temperature was 370 ºC
  - The heat required to bring the wood up to pyrolysis temperature was determined by integrating its temperature dependent specific heat
  - The heats of storage and transit were determined by multiplying the difference between the measured surface temperature and the pyrolysis temperature by average specific heats of char and volatiles
  - Directly measured char fraction is used in the calculation

Summary (4)

- The calculated hg was compared with the measured one. The agreement was good.
- It should be possible for CFD model to predict fire growth in an enclosure if h_g as a function of char depth measured in laboratory is used. Material thickness and rear boundary conditions must be the same.
- The model needs to recognize when conditions are reached that do not support full flame coverage of the surface.